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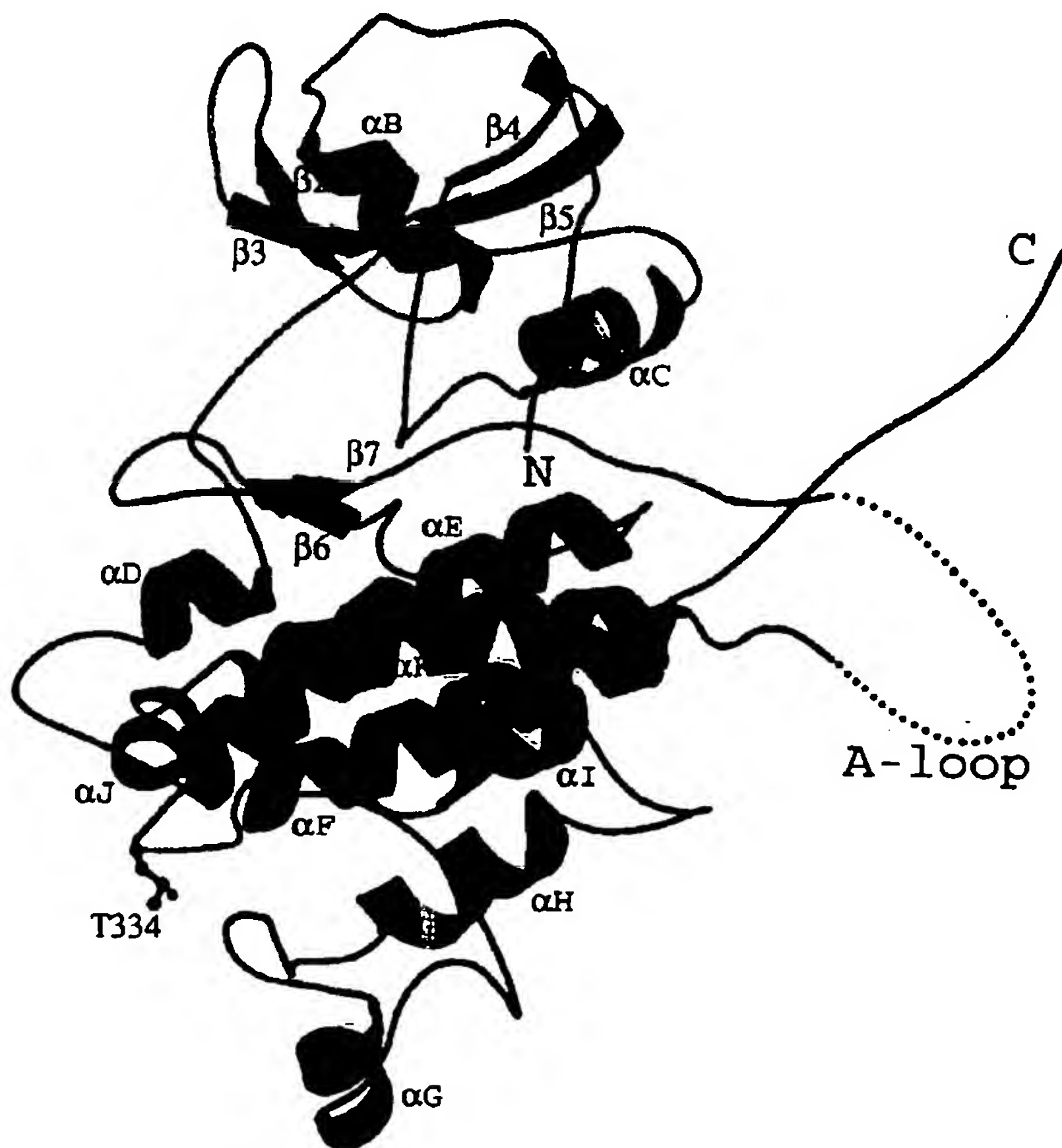
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(54) Title: CRYSTAL STRUCTURE OF MITOGEN-ACTIVATED PROTEIN KINASE-ACTIVATED PROTEIN KINASE 2 AND BINDING POCKETS THEREOF



(57) Abstract: The invention relates to crystalline molecules or molecular complexes that comprise binding pockets of mitogen activated protein kinase activated protein kinase 2 (MAPKAPK2) or its homologues. The invention also relates to crystals comprising MAPKAPK2. The present invention also relates to a computer comprising a data storage medium encoded with the structural coordinates of MAPKAPK2 binding pockets and methods of using a computer to evaluate the ability of a compound to bind to the molecule or molecular complex. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for, design and optimize compounds, including agonists and antagonists, which bind to MAPKAPK2 or homologues thereof.

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